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3-D Numerical Study of Effect of Urea Injector Location and Intake Cone Geometry on SCR Performance

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Abstract

In response to current strict laws aiming to reduce motor vehicle emissions, more and more research projects are being carried out in order to enhance the flow of automotive catalysts. There have been substantial efforts to further refine the SCR technology (selective catalytic reduction) for diesel-powered vehicles. Furthermore, only a little distance from the catalytic input between the exhaust system is available for a mobile SCR system. This therefore leads to an insufficient urea residence period, and evaporation and thermolysis at the catalyst entry cannot therefore be completed. This can lead to substantial secondary ammonia and isocyanic acid emissions. Therefore, fast thermolysis, effective ammonia blend with exhaust gas and reduction of ammonia slip are crucial factors for the deployment of SCR technology on cars. The Computational Fluid Dynamics (CFD) approach is used for optimizing the exhaust gas flow inside the existing catalyst by changing intake cone designs which is intended to be used on Euro VI/Bharat Stage-VI emissions legislation compliant heavy-duty diesel engines in India. This study is divided in to two parts. The first part of the study deals with finding the optimized ammonia injector location, and in the second part, the proposed inlet cone design's flow velocity uniformity index is estimated and compared with that of the existing SCR catalyst model.

Keywords: Nitrogen oxide (NO_x), Selective catalytic reduction, Uniformity index, Ammonia slip, Computational fluid dynamics, Emission control.

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1. Introduction

With the rapid growth of automobiles on the road, many environmental issues such as pollution and smog formation are arising. To counter the problem, the world's first vehicle emission norms were enacted by the California Air Resource Board (CARB) in 1963 in Los Angeles. Later, most countries in the world followed the enactment of their own emission norms. From April 2020, the Government of India has implemented BS-VI norms for petrol and diesel vehicles nationwide.

Due to increased public awareness, environmental safety is one of the most popular research topics these days. Continuous efforts are being made to decrease pollution and create environmentally friendly procedures in order to attain this goal. The environmental pollution caused by marine diesel engine exhaust emissions, particularly nitrogen oxide (NO_X) emissions, is severe [1, 2]. In comparison to NO_X, the automobile Diesel engine produces a lot of carbon monoxide (CO), carbon dioxide (CO_2), and hydrocarbon (HC) as exhaust emissions. The NO_X emissions from a marine diesel engine, on the other hand, are more harmful [3]. As a result, several national and international organizations have implemented and enforced stringent NO_X emission regulations in order to reduce ship exhaust emissions [4]. The International Maritime Organization (IMO) has implemented Tier III NO_X emission regulations across North America, the West and East Coasts of the United States, and the Caribbean in 2016. In the future, it will be applied in the North Sea and the Baltic Sea. [5]. High pressure fuel injection and Exhaust Gas Recycling (EGR) systems are preferred for reduction of NO_X emissions, but advanced and improvements are needed to tackle difficulties caused by poor engine performance and steadily growing stringent vehicle emission regulations [6]. "Exhaust gas treatment is the most practical and straightforward option. Due to its high NO_X reduction effectiveness, cost-effectiveness, and better fuel economy, Selective Catalyst Reduction (SCR) is the most popular after-treatment method used to meet the latest NO_X emission regulations [7]".

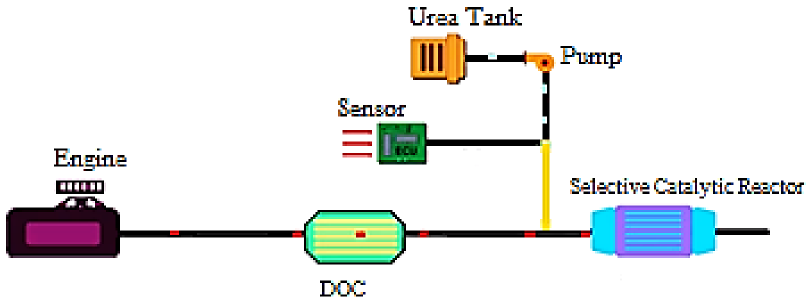


Figure 1.
Schematic layout of SCR system.

Figure 1 shows the schematic layout of SCR system, injector inject the control quality of water/urea solution at inlet of SCR. This solution turn into ammonia (NH3) and react with NO_X in flue gas and produce water drops and Nitrogen gas as follow,

$$NO+NO_2+2NH_3 \longrightarrow 2N_2+3H_2O \qquad (1)$$

The SCR system is capable of reducing about 90% of NO_X [8] but there are a few issues with the SCR system, like improper urea water solution (UWS), ammonia slip, UWS and exhaust gas moisture etc. [9]. Injection of UWS is (32.5 percent urea) into exhaust gas [10, 11]. "If ammonia is abundant in comparison to NO_X at the vicinity of the SCR catalyst, there will be un-reacted ammonia in the exhaust gas after the catalyst. This causes ammonia slip and is undesirable from an environmental standpoint. If this happens, urea injection should be optimised in terms of geometry and operating circumstances early in design process [12]".

The performance of SCR system depends on many parameters, including the position of urea injector, inlet cone design, temperature of exhaust gas, quality of urea flue gas mixture etc. The position of a urea injector influences the effectiveness of the urea-water SCR system by quick ammonia mixing, evaporation and heat drifting. The optimized distances between the urea injector and the ammonia entrance significantly increases the uniformity of ammonia [13]. Due to improper injection, urea or its by product is deposited on the inner surface of the SCR and it leads to increased back pressure [14]. When temperature is above 200°C, NH_3 decomposes completely and it will improve NO_X conversion efficiency [15].

With the detailed examination of past investigations, it is crucial that urea be completely converted into ammonia for optimum NO_X reduction by adequate thermolysis and hydrolysis of urea. However, a small distance between urea injection and the catalyst entry is possible with the mobile SCR system. This leads to a degradation of ammonia and HNCO that causes a considerable loss of performance and deposition of urea. Therefore, in terms of its place at an early stage of design, urea injection should be optimized. Uniform flow distribution at the entrance of the monolith structure plays a major role in the complete conversion of NO_X. This depends upon the intake cone geometry of the catalyst. In this paper, changes in flow uniformity in axi-symmetric catalysts due to different intake cone designs are explored in depth. In the first part of the study, the injector location for improving conversion efficiency was analysed, and the second part of the study focused on optimizing the intake cone geometry for increasing velocity uniformity index.

2. Review of Recent Work

To improve the performance of various experimental and numerical studies have been performed by researchers. Mehdi, et al. [16] developed a computational model to investigate the interaction of urea droplets with exhaust gas and its impacts. It shows the uniformity of flow velocity, uniformity of ammonia distribution in the catalyst, and temperature distribution are among the performance parameters. Flow maldistribution at the catalyst's front face causes bigger ageing effects in these zones, resulting in worse overall species conversion efficiency. Lu, et al. [17] proposed a new mixer design for diesel engines. It was observed that by employing this mixer, urea droplets fully mixed with flue gas and increased NOX conversion efficiency, with velocity uniformity index and ammonia uniformity index of 0.98 and 0.95, respectively. Budziankou, et al. [18] studied the impact of urea droplets on the wall of the exhaust pipe and the formation of liquid film experimentally on an engine test bench. The liquid film formation is observed by IR thermography. This liquid film is responsible for creating the back pressure, which ultimately reduces the engine efficiency. Similar results were recorded by Qian, et al. [19]. Hence, a proper urea injection system is important. Jain, et al. [20] performed the numerical analysis and observed that the injection angle had a key impact on urea decomposition. Chen, et al. [21] performed experimental and numerical analysis to reduce the urea deposits formation. Studies show that liquid film formation can be reduced by proper urea injection pressure, injection angle, and injecting the urea with high turbulence intensity. Chen and Williams [22] used CFD-based intake cone design to optimise flow distribution. The flow distribution of the catalytic converter across the substrate should be uniform, because it provides more surface area for chemical reactions. Figure 2 depicts a substrate whose face was eroded as a result of non-uniform exhaust flow. The regular flow distribution also influences the durability of the substrate and support mat [23].

Figure 2.
Substrate erosion caused by non-uniform flow [23].

Experimental optimization of catalytic converter design parameters is extremely expensive and time-consuming. Several prototypes need to be built for experimental testing with various geometry during the design phase. Geometric variations have a huge impact on the flow inside a catalytic converter. These models must be extremely accurate. The stereo-lithographic production of CAD data plastic models has proven to be a precise approach and an effective tool for internal flow device testing, but it’s a time-consuming and expensive method. As a result, using a CFD approach to design catalytic converters is more viable [24]. Hence, in order to study the effect of injector location and inlet cone geometry on SCR performance the CFD approach is adopted. 3D SCR CAD model is created on SolidWorks software and imported in ANSYS Fluent for further analysis.

3. Methodology

As discussed in the previous section, this work consists of two different types of analysis. In the first part of the study, the injector location for improving the conversion efficiency was analysed. While in the second part of the study is focused on optimizing the intake cone geometry for increasing velocity uniformity index.

3.1. Part 1. Injector Location

Initially, in this exhaust pipe system, the injector location was proposed at first bend. But at the bend location the installation of injector is very difficult and also the non-uniform flow distribution and formation of eddies may occur in that vicinity. That may cause high energy loss and mal-distribution of urea which will result in less conversion efficiency. So, to find out optimized position of urea injector, exhaust pipe flow simulations were performed at four different operating load conditions of engine. This is because convergence can be hard to achieve if all options, such as second-order numerical schemes, had to be employed from the beginning of the simulation.

3.1.1. Geometry and Mesh Generation

The models used for optimizations are created in the CAD package and the computational model is created in CFD. The volume mesh consists of tetrahedral elements. 5 prism layers of 1 mm thickness are utilised along the walls of the pipe to enhance accuracy in border layers, as shown in the Figure 3. Grid dependent study was done to see the effect of mesh size and element size were found to be 2mm effective.

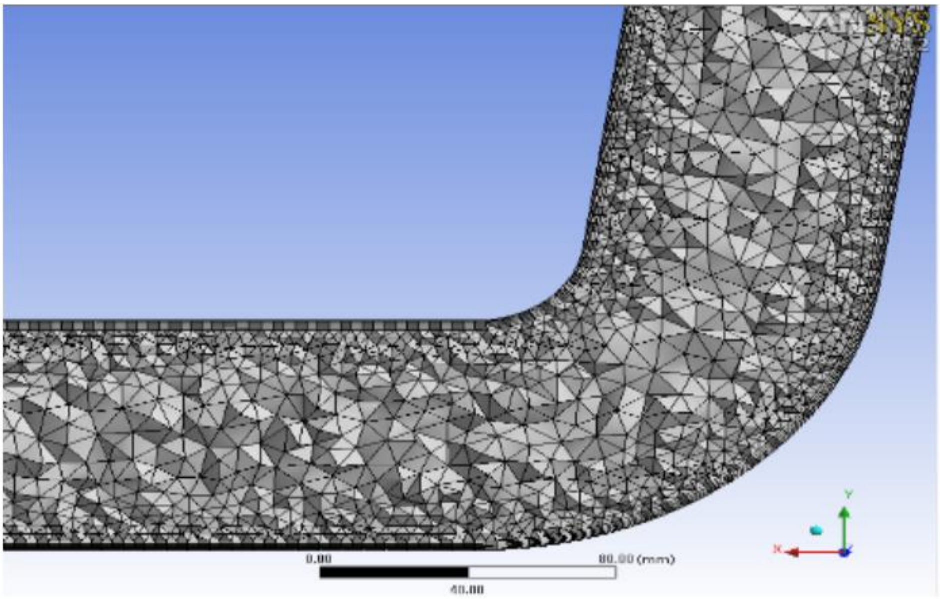


Figure 3.
Exhaust pipe meshing.

3.1.2. Boundary Conditions

The inlet plane of the CFD domain was defined as an 'inlet boundary' with a uniform axial velocity prescribed corresponding to the actual mass flow rate in each flow condition. For the first case A, the inlet velocity is taken as 82.78 m/s at 1400rpm which was measured on test bed for particular engine. At the exterior walls of the exhaust pipe heat transfer due to thermal conduction and convection was taken into account. The material considered for the conduction was steel with thermal conductivity of 16.27 W/mK. Convection was taken into account by heat transfer coefficient of 7.9 W/m2K.

3.2. Part 2. Intake Cone Design

Intake cone geometry and design are the main factors that determine how uniformly exhaust gas flow is distributed throughout the substrate of the catalyst. As a result, the catalytic converter's conversion efficiency is determined by the intake cone design. In other words, the intake cone geometry determines the catalytic converter's emission conversion performance. The Computational Fluid Dynamics (CFD) method is used to predict and optimize the flow distribution of a SCR catalyst. The current model is used to investigate flow distribution.

3.2.1. Uniformity Index Calculation

In order to examine the effect of flow distribution over the substrate, velocity contour plot is considered at three different sections for the given model. The uniformity index (γ), is calculated for three different sections as follows:

$$\gamma = 1 - \frac{A_i}{2A} . n \left[\left| \frac{u}{\bar{u}} - 1 \right| \right] \quad (2)$$

Where, u is the local velocity; $\bar{u}$ is the mean gas flow velocity of the cross section; N is the total number of cells; A is the cross-section area of substrate; Ai is the flow area of cell "i" and "i" one of the "nth" cells.

3.2.2. Flow Uniformity Acceptance Criterion

The volume of SCR substrate must be at least 90% of the engine swept volume to achieve excellent emission conversion efficiency irrespective of precious metal loading. Intake cone design for SCR system will be accepted as successful if only acceptance criterions applied in major automotive manufacturers are satisfied. The uniformity index should be $\gamma \geq 0.94$.

3.2.3. Geometry and Mesh Generation

For simulation a commercially available catalytic converter with circular cross section was modelled and mesh was generated. The specification of the substrate and coating are listed in Table 1. The volume mesh consists of 774048 non uniform hexahedral cells. The mesh is exported in the CFD package and the skewness and other mesh quality criteria were checked using check mesh utility. The computational meshed model is shown in Figure 4.

Table 1.
Substrate specifications.

Material	Diameter	Length	Cell density	Wall thickness	Coating
Cordierite	6.77"	17"	400cpsi	7 (mil)	V_2O_5

Note:" means inch (British imperial dimension).

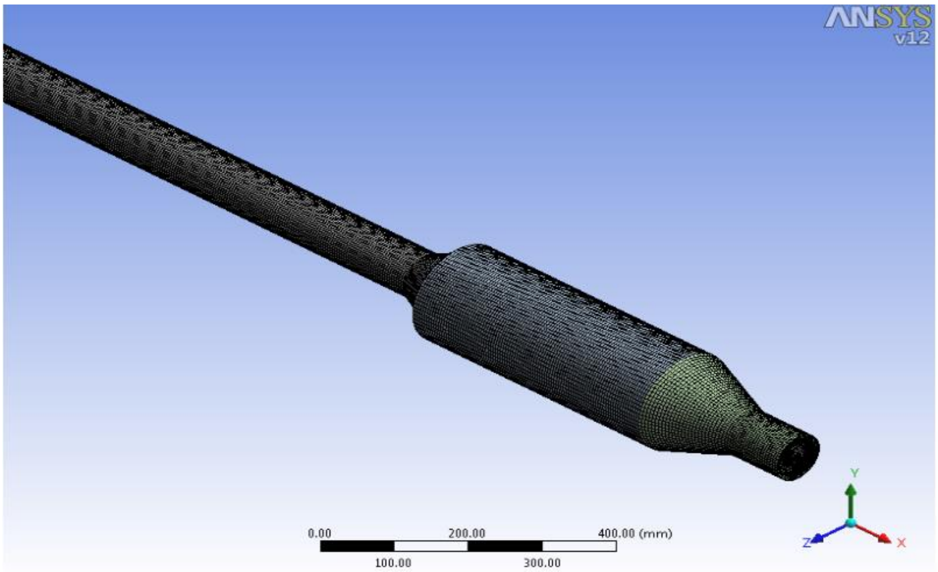


Figure 4.
Existing SCR meshed model.

3.2.4. Proposed Intake Cone Geometry

The CAD model for four different cones are created in CAD Package as shown in Figure 5. The volume mesh consists of non-uniform tetrahedral cells for all the four cones. Porous medium flow resistance formulae were input to the model for the prediction of velocity distribution across the catalyst monolith. The mesh containing 6.77"*12", 400cpsi unwashcoated substrate was modeled and cell density was kept 14400.

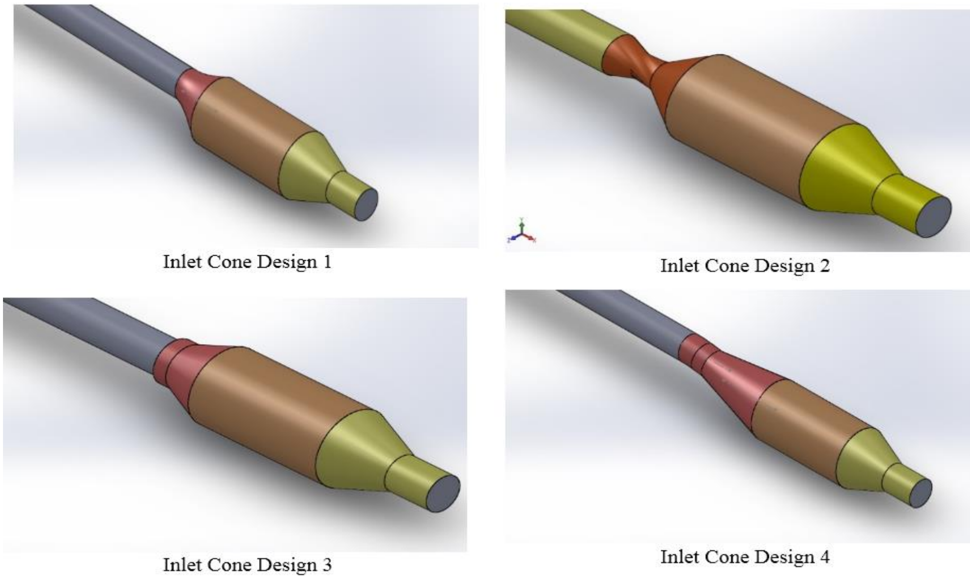


Figure 5.
Proposed inlet cone geometry design.

As seen in Figure 5 above, in the intake cone design 1, the intake cone shape was made divergent with little downward offset. In the intake cone design 2, to create swirl motion, the intake pipe was twisted and the intake cone shape was kept divergent. In intake cone design 3, the catalyst diameter was increased at the inlet section along with the cone length. In the intake cone design 4, the pipe was bent downward to create a downward offset and the intake cone length was increased.

Table 2.
Exhaust conditions of diesel engine for different loading cases.

Lading Case	Speed (rpm)	Inlet Velocity of Exhaust Gas (m/s)	Outlet condition (Pressure outlet)	Temperature of exhaust gas at inlet (°C)
A	1400	82.78	Const.	480
B	1730	48.70	Const.	350
C	1730	66.99	Const.	400
D	2060	76.59	Const.	375

3.2.5. Boundary Conditions

For CFD simulations inlet boundary conditions, an engine test bench experiment data was chosen. Four different operating conditions (load cases) are considered for simulations as given in Table 2 and remaining boundary conditions considered for CFD analysis are as shown in Table 3.

Table 3.
Boundary conditions.

Parameter	Setup for Existing Model and Proposed Cone Design
Inlet Conditions	As mentioned in Table 2.
Outlet Conditions	Pressure outlet
Flow Properties	3D, Steady state, turbulent
Fluid Properties	Nitrogen, incompressible
Turbulence model	Standard k-e model
Porous medium coefficients	V_R^*=2.566e7 [1/m^2], I_R^*=3.67 [1/m]
Fluid boundaries	No slip wall
Porous material boundaries	Slip wall
Turbulent intensity	Inlet =10% Outlet=5%
Mesh type and mesh number	Hexahedral, 774048

Note: *-Manufacturers defined values

4. Results and Discussion

The effect of inlet injector location and inlet cone geometry of SCR performance is discussed in following subsections.

4.1. Effect of Injector Location

The estimated flow fields are displayed in various sections of the current pipe. The velocity contour for load case A is shown in Figure 6 in the x-direction at a symmetric cross-section parallel with the inlet flow direction. For the case A, the flow separation occurs at the bends which result in high energy loss. Flow separation is highly undesirable because it will lead to improper mixing of UWS with exhaust gas. After the bend section of pipe, the flow is getting more uniform as the flow advances in x-direction.

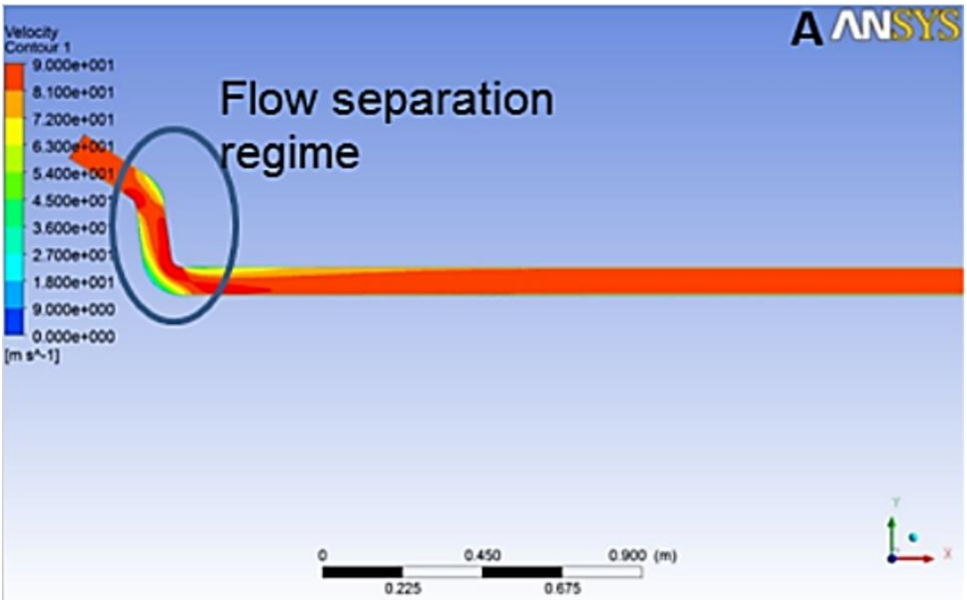
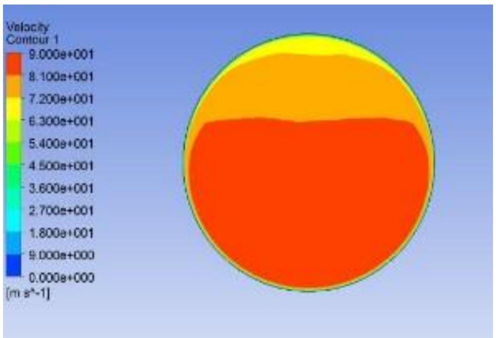
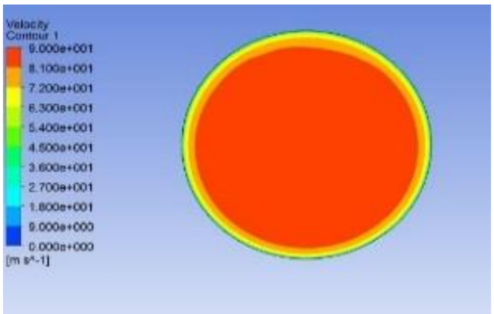
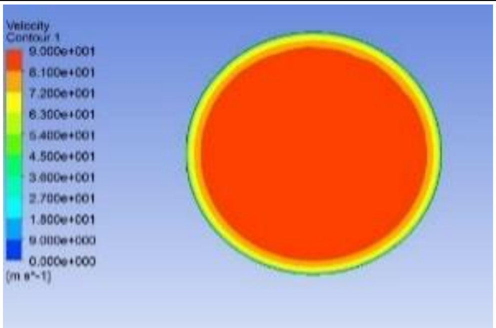


Figure 6.
Velocity contour of exhaust gas.

CFD plots are taken upstream of monolith entrance at 5.5, 14.5 and 24 (termed 5.5D, 14.5D and 24D respectively) times exhaust pipe diameter to visualize the velocity contour in more detail. The CFD plot for case A, at 5.5D, 14.5D and 24D are shown in the Table 4. As the flow advances toward the outlet, it gets fully developed which will help for better atomization of urea droplet and uniform mixing with exhaust gas. The position of the UWS injector is between 5.5D and 14.5D to achieve improved mixing and evaporation with the exhaust gas. However, it may be seen that more than 14.5D upstream injector position shows a small improvement in ammonia concentration uniformity.

When the distance between the injector and the monolith exceeds certain criteria, the majority of the urea droplets have evaporated and are fully mixed up before the SCR catalyst. These facts demonstrate that increasing the distance between the injector and the SCR catalyst over 14.5D of the exhaust pipe diameter upstream in the study is pointless.

Table 4.
CFD plot at different sections of pipe (Case A).

Section	CFD Plot	Remark
24D		The flow is not fully developed and uniform in this segment, which might result in improper urea mixing and lower conversion efficiency.
14.5D		The flow is fully developed in this segment, allowing for better mixing of urea droplets and exhaust gas. The distance is also greater from the monolith face, which increases resident time for interaction, increasing droplet evaporation and therefore improving atomization.
5D		Flow uniformity increased a bit compared to previous section.

4.2. Effect of Inlet Cone Geometry

CFD Simulations were performed for four different operating conditions (as per Table 3) on four different inlet geometry designs along with existing SCR model to find out the uniformity of gas velocity (γ) at entrance and inside the monolith and pressure drop across the monolith were studied.

4.2.1. Existing SCR Catalyst Model

The flow in the catalyst is determined by geometric configuration and the flow resistance characteristic of the substrate. The velocity contour map for existing SCR model for case B, in the x-direction at a symmetric cross-section parallel to the direction of the inlet flow is shown in Figure 7.

The velocity of exhaust gas flow from upstream to downstream in the centre of the pipe has been shown to be quite unequal. The velocity at the centre of the exhaust pipe is high. When the flow enters the porous zone, it aligns with the channel direction. At the entrance of the porous zone, the uniformity of flow is low. At the end of the Intake Cone, a recirculation zone is formed, which is highly undesirable. Near the wall, substrate velocity is very low, which reduces the uniformity of flow. The uniformity index of velocity for existing model was calculated as 0.84 at middle portion of catalyst.

The existing model was also tested on the test bed for NO_X conversion efficiency as shown above in Figure 8. The NOx conversion efficiency was found 80.82%. Pre-SCR Cat NO_X reading was 9.746 gm/kW.hr and Post Cat it was 1.869 gm/kW.hr.

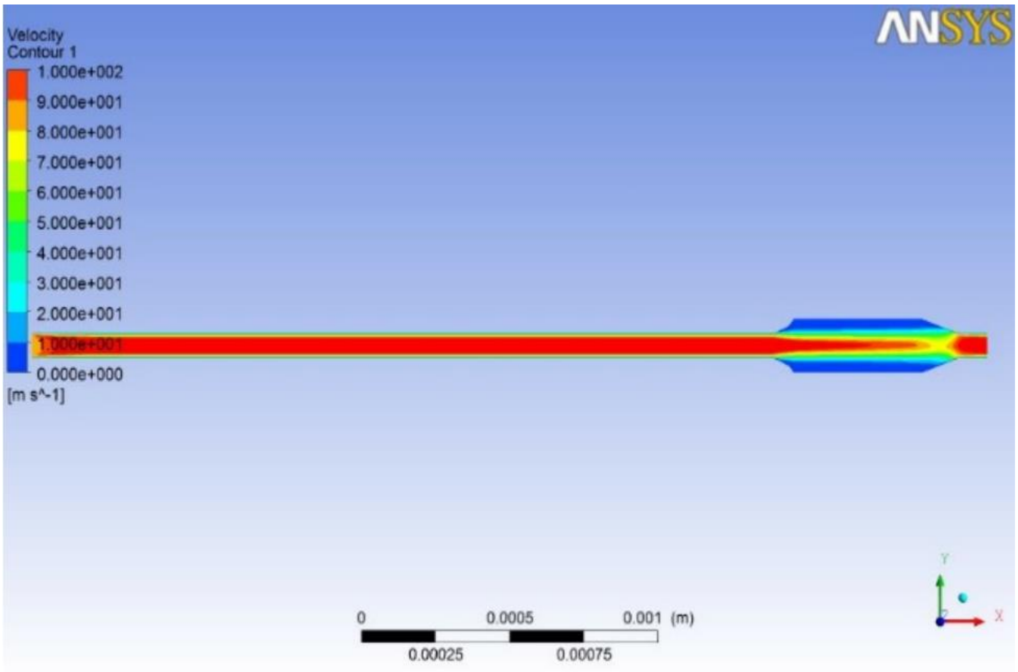


Figure 7.
Velocity contour for existing SCR model.

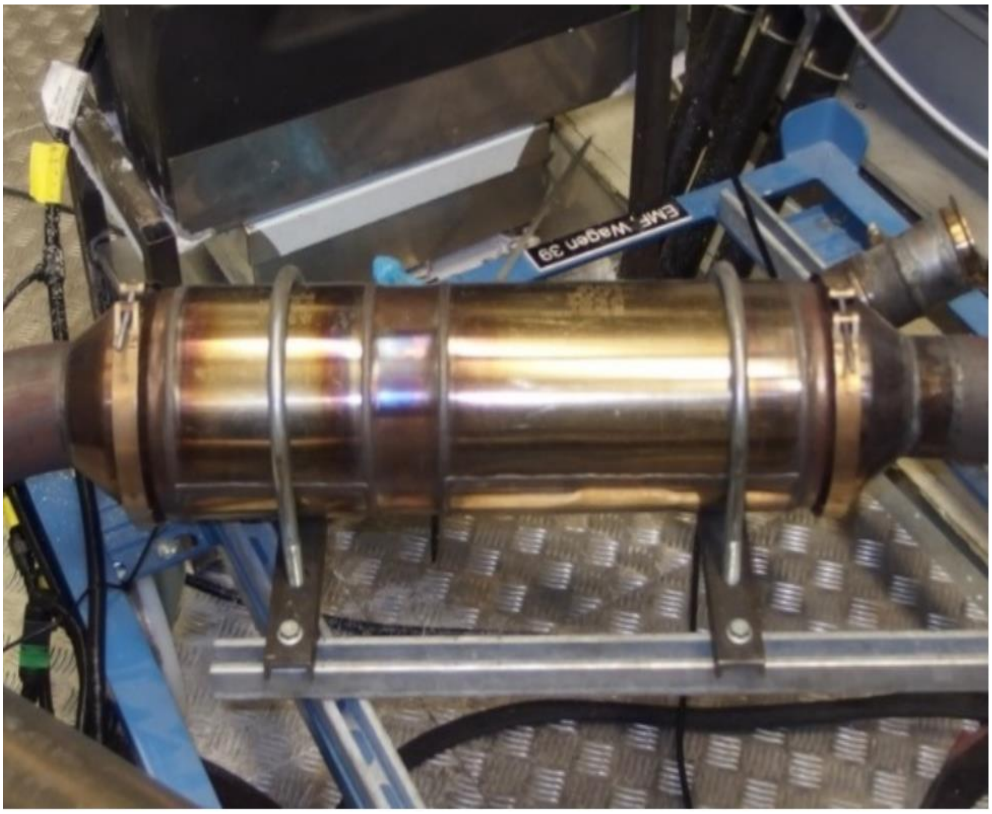


Figure 8.
SCR experimental set up.

4.2.2. Intake Cone Design 1

The contours of the velocity for intake cone design model 1 is shown in Figure 9. It is seen that, the flow velocity at the centre of the pipe is high. When the flow enters the porous zone, it aligns with channel direction. At the entrance of porous zone flow velocity slightly reduces and after entering into porous zone it decreases along the length of catalyst. As the cone is eccentric to the axis of substrate, the flow deviates to the only one side, which is giving non uniform velocity distribution.

In the intake cone end, recirculation zone are formed downward side of intake cone, which is highly undesirable. Near the wall of substrate velocity is very low and which reduces the uniformity of flow.

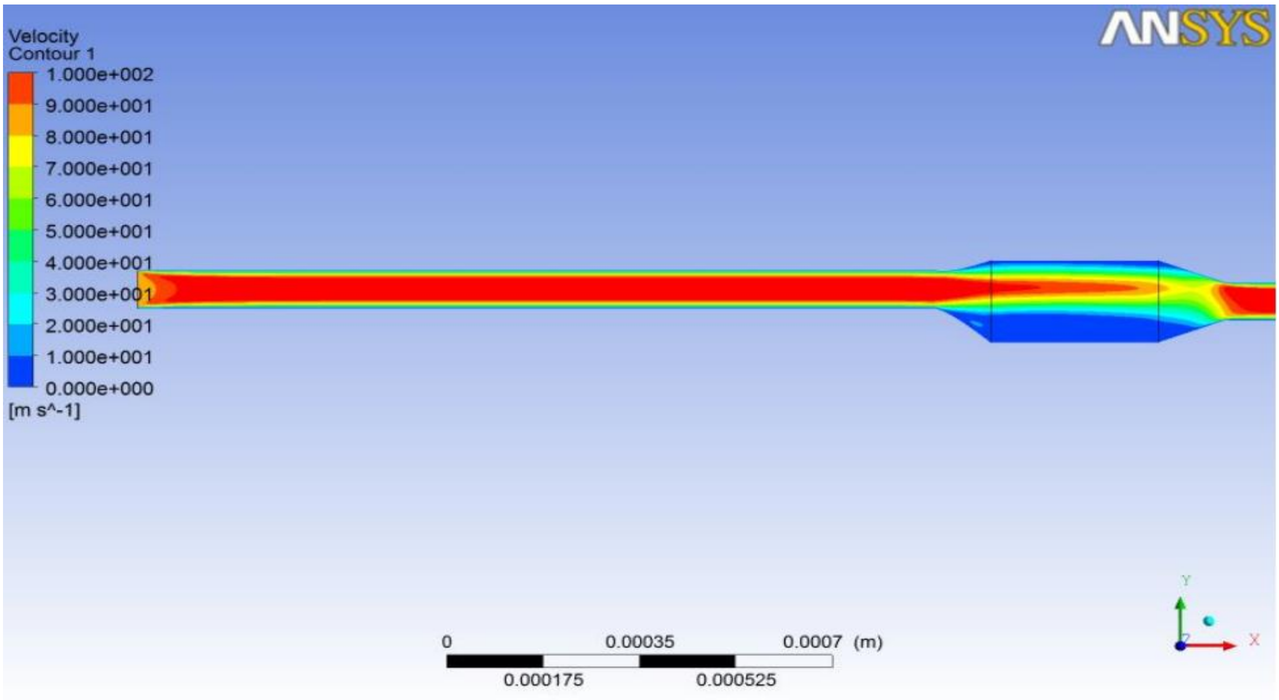


Figure 9.
Velocity contour for cone design 1.

4.2.3. Intake Cone Design 2

For the intake cone 2 as shown in Figure 10, velocity is very higher at the centre of the substrate, which results in non-uniform distribution of flow. As the flow enters in porous zone, it aligns with the channel direction and flows with maximum velocity at centre of substrate. The flow is separated at the wall of cone and forms small recirculation zones. The flow uniformity increases slightly at centre compared to first intake cone.

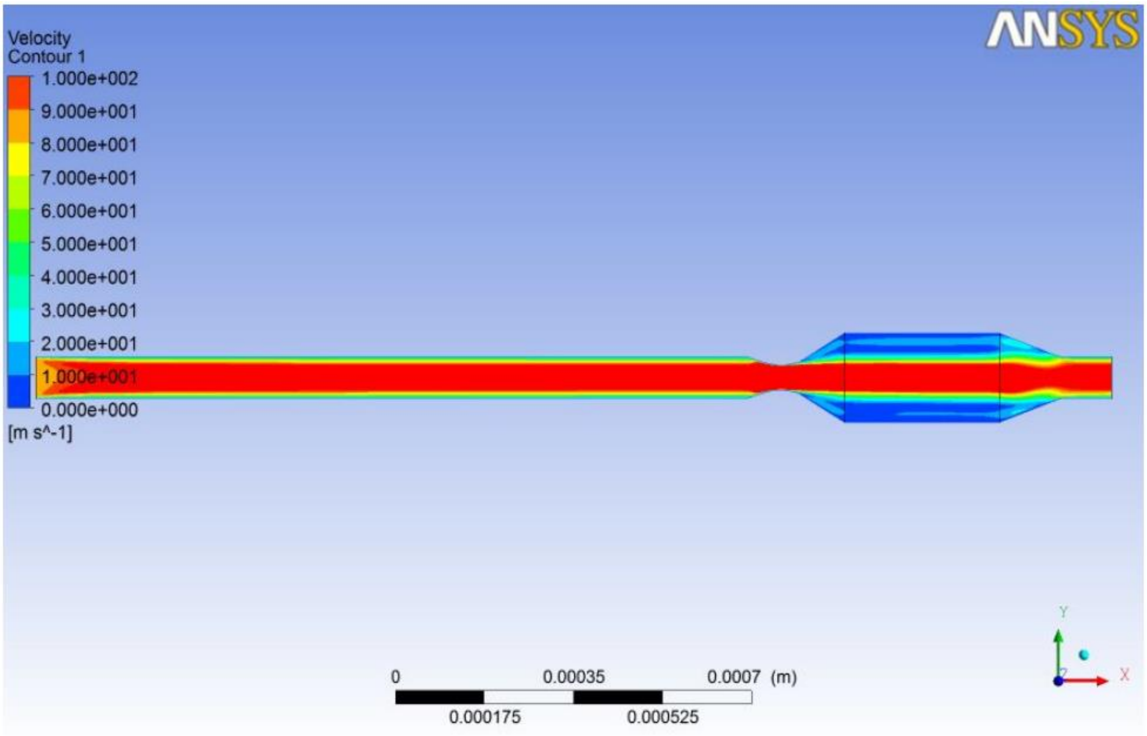


Figure 10.
Velocity contour for cone design 2.

4.2.4. Intake Cone Design 3

For intake cone 3 Figure 11, the flow is more uniform because of the greater entrance angle inside the catalyst. In addition to the slight velocity reduction at the cone wall, the flow spreads evenly along the length of the substrate.

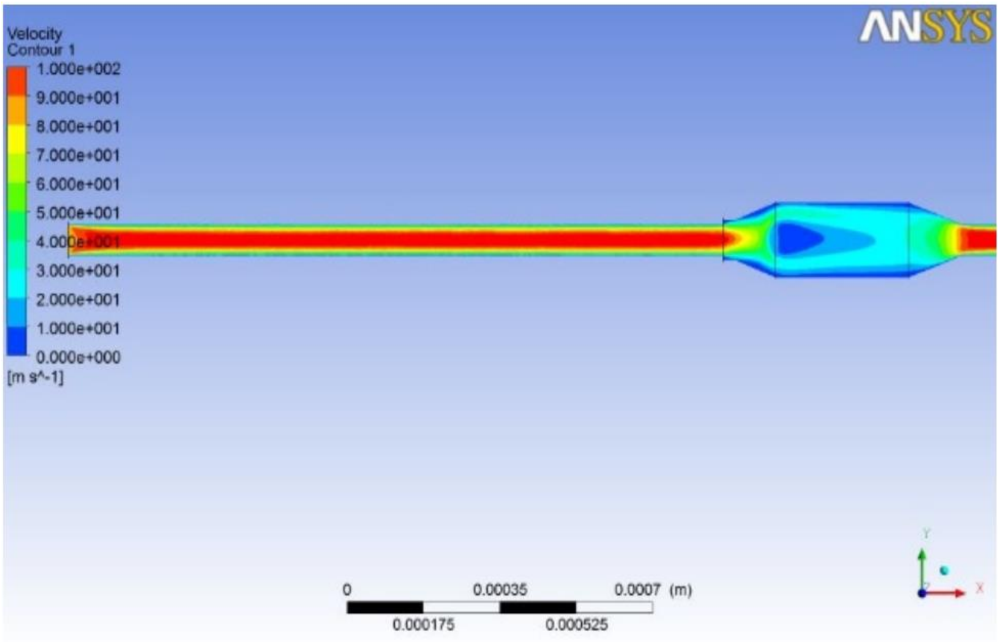


Figure 11.
Velocity contour for cone design 3.

4.2.5 Intake Cone Design 4

For intake cone 4 Figure 12, the flow is uniformly spread all over the substrate as it enters. The small flow separation takes place at the start of the cone wall, which reduces as the flow advances. The uniformity of flow is constant throughout the substrate. Higher flow uniformity was observed in this intake cone design.

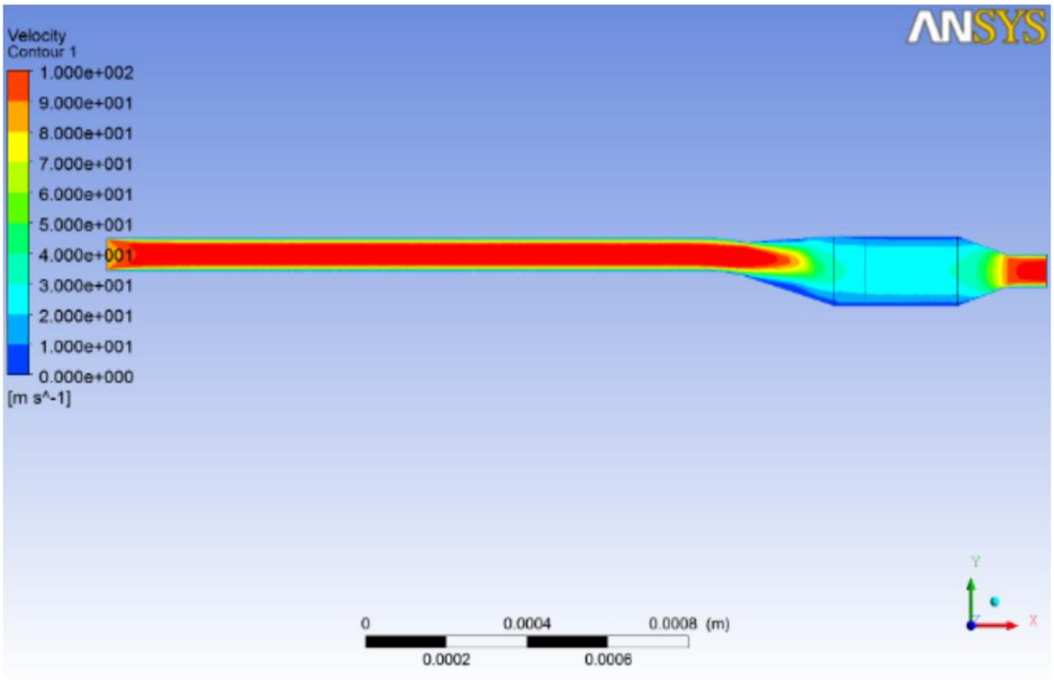


Figure 12.
Velocity contour for cone design 4.

4.2.6. Velocity Uniformity Index

The velocity uniformity index and exhaust gas mixture in the axial direction at the catalyst inlet has a direct impact on catalyst conversion efficiency and utilization rate. The Figure 13 shows velocity contours for existing SCR model and proposed intake cone design 4 at middle of catalyst. The flow velocity uniformity index for existing SCR model and proposed intake cone design 4 were calculated as 0.84 and 0.96 respectively.

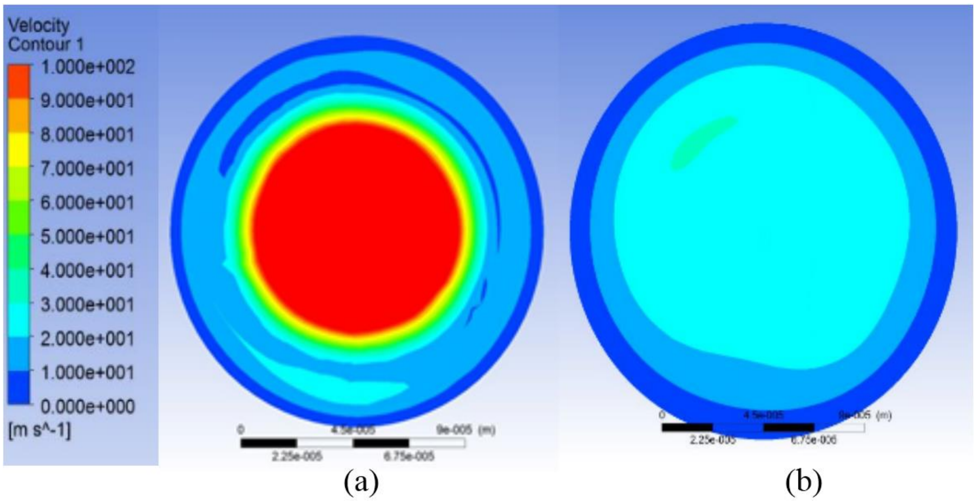


Figure 13.
Flow velocity contour maps at mid-section of the catalyst (a) existing SCR model, (b) Intake Cone design 4.

5. Limitations of the Study

In this study, the CFD analysis is carried out considering ideal conditions. Because of the numerous simplifications and approximations employed in numerical simulations, there are several possible causes of inaccuracy. CFD simulations are prone to convergence problems and require an extremely fine mesh. The proposed intake cone geometry design can also lead to develop any other problems related to manufacturing and fabrication. As mentioned in earlier sections, the experimental analysis of catalytic converters is costly and time-consuming, hence proposed cone designs are not validated by experimental analysis.

6. Conclusion and Future Work

In this study, three-dimensional numerical modelling and flow simulation have been performed for the design optimisation of the SCR catalyst system in heavy duty diesel vehicle applications to find the optimum injector location, flow distribution inside the catalyst and other design parameters. The top results are listed below.

i. When the injector is located between 5.5 and 14.5 times exhaust pipe diameter (D) upstream, the flow uniformity increases due to uniform flow distribution in the pipe.
ii. To accomplish the maximum conversion efficiency, the exhaust gas flow in the exhaust pipe and the frontal part of the substrate must be uniform. The key parameter that decides the flow uniformity in the substrate is the intake cone design of the catalyst. The exhaust flow uniformity was increased by optimizing the intake cone design step by step, and finally, the intake cone was accepted as the best one.
iii. CFD predictions showed that the uniformity index of the proposed intake cone design 4 is 14.28% more as compared to the base model.

This work can be extended by including the analysis of the effects of injection pressure, number of injector holes, injector angle and direction of injection in the SCR system. Also, by adding honeycomb like flow straighteners in the exhaust pipe, the flow uniformity can be further improved. Further flow distribution analysis can be done by changing the parameters of honeycomb flow straighteners.

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